Wednesday Morning, September 21, 2022

Fundamentals

Room Great Lakes B - Session FM-WeM1

Fundamentals - Secondary Ion Formation I

Moderator: Andrew Giordani, Procter & Gamble Company

8:40am FM-WeM1-1 Improving Uranium Particle Analysis by SIMS using O₃-, *Evan Groopman, T. Williamson, D. Simons*, National Institute of Standards and Technology (NIST) INVITED

We have investigated the use of negative molecular oxygen primary ion beams (i.e., O_2^- and O_3^-) to determine the benefits of using such beams for U particle SIMS analyses. Typically, O⁻ is the most practical negative primary ion species for both age dating and uranium isotopic analysis with the conventional duoplasmatron ion source. Molecular $O_2^{\mbox{-}}$ and $O_3^{\mbox{-}}$ are produced in greater abundance in newer RF plasma sources, making them viable primary beam species for these analyses. We used two particulate samples of known mass, IRMM CRM 2329P and inkjet printed deposits, to compare the useful yields of U⁺, UO⁺, and UO₂⁺ ions under Köhler bombardment from O^{-} , O_{2}^{-} and O_{3}^{-} . We also investigated the effects of substrate chemistry and primary species on the Th/U relative sensitivity factor by measuring particles of NIST CRM U900 on graphite and silicon. We determined that by using an O_3^- beam, the ionization yield of uranium can be increased by a factor of approximately two over an O⁻ beam, up to 4.7%, a substantial improvement which positively impacts measurement precision and detection limits. We also found that O3⁻ reduced instrumental mass fractionation and matrix/substrate effects relative to the other negative ion beams. Particle measurements using O_3^- were improved in every respect compared to conventional O⁻ beam analyses. With the use of increasingly common RF oxygen sources, the precision of U particle measurements can be improved by using O3⁻ primary ions without the need for additional changes to standard operating procedures.

9:20am FM-WeM1-5 Surface Properties of Ionic Liquids: A Mass Spectrometric View Based on Soft Cluster-Induced Desorption, *Karolin Bomhardt*, *P. Schneider*, *T. Glaser*, *M. Dürr*, Justus-Liebig-University Giessen, Germany

lonic liquids (IL) feature a large technological potential, e.g., in catalysis or as designer solvents; with respect to their bulk properties, they have been intensively investigated. However, since in most applications the interaction proceeds via the surface of the IL, e.g., in the case of catalytic reactions, the surface properties are of equal or even higher interest.

Here we show the application of Desorption/Ionization Induced by Neutral SO₂ Clusters (DINeC) [1] in combination with mass spectrometry (MS) for the investigation of the molecular composition of the surface of IL. Clear and fragmentation-free spectra of the cations and anions present in the sample are obtained after DINeC from bulk and thin film samples of IL. Based on both softness [2] and surface sensitivity [3] of DINeC-MS, accumulation of either cations or anions was discriminated on the surface of bulk IL, depending on the molecular structure of the IL components. In particular, cations with long alkyl chains were found to aggregate on the surface, but this tendency is the more reduced the larger the respective anion is; in the case of larger anions and smaller cations, the effect is found to be even reversed.

For thin layers of IL, the ratio between cations and anions as detected in the mass spectra is further influenced by the surface of the substrate; structural inhomogeneities such as the formation of islands of bulk material as well as the dynamical behavior of the thin film layer are deduced from the temporal evolution of the mass spectra and the relative intensities of cations and anions.

References:

[1] C. R. Gebhardt, et al., Angew. Chem., Int. Ed. 48, 4162 (2009).

[2] M. Baur, et al., Rapid Commun. Mass Spectrom. 28, 290 (2014).

[3] A. Portz, et al., Biointerphases 15, 021001 (2020).

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